

(FILE 'HOME' ENTERED AT 10:03:11 ON 10 DEC 2003)

FILE 'REGISTRY' ENTERED AT 10:03:20 ON 10 DEC 2003

L1 STRUCTURE UPLOADED
L2 2 S L1
L3 376 S L1 FULL

FILE 'CAPLUS' ENTERED AT 10:04:02 ON 10 DEC 2003

L4 379 S L3
L5 325 S L4 AND PY<1999

=> s 15 and DTPA
8046 DTPA
L6 191 L5 AND DTPA

=> s 15 not 16
L7 134 L5 NOT L6

=> d 1-50 bib abs

L7 ANSWER 1 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1998:499082 CAPLUS
DN 129:169697

TI Methylation of Tethered Thiolates in [(bme-daco)Zn]2 and [(bme-daco)Cd]2
as a Model of Zinc Sulfur-Methylation Proteins
AU Grapperhaus, Craig A.; Tuntulani, Thawatchai; Reibenspies, Joseph H.;
Darensbourg, Marcetta Y.
CS Department of Chemistry, Texas A&M University, College Station, TX, 77843,
USA
SO Inorganic Chemistry (1998), 37(16), 4052-4058
CODEN: INOCAJ; ISSN: 0020-1669
PB American Chemical Society
DT Journal
LA English
AB The dimeric dithiolate complex [1,5-bis(mercaptoethyl)-1,5-
diazacyclooctanato]zinc(II), [(bme-daco)Zn]2 or Zn-1, and its Cd analog,
Cd-1, were studied as models for the active site of Zn-dependent
methylation proteins. The key issue addressed was whether alkylation of a
thiolate in a relatively rigid tetradentate ligand would result in
coordination of the thioether product to the metal. From 1H and 13C NMR
spectroscopy and similar reactivity toward alkylating agents, the newly
synthesized Cd complex, Cd-1, probably is isostructural with the
previously reported Zn-1 complex, which is known from x-ray crystallog. to
be dimeric in the solid state (Tuntulani, T.; Reibenspies, J. H.; Farmer,
P. J.; Darensbourg, M. Y. Inorg. Chem. 1992, 31, 3497). Iodomethane
reacts with Zn-1 in hot MeOH/MeCN to produce a thioether which dissocs.,
replaced by coordination of iodide in the pseudo-tetrahedral complex,
(Me2bme-daco)ZnI2 or Zn-2. Complex Zn-2 crystallizes in the triclinic
space group P.hivin.1 with a 7.911(2), b 10.675(2), c 12.394(2) .ANG.,
.alpha. 75.270(10), .beta. 75.270(10), .gamma. 82.12(2).degree., and Z =
2. An analogous reaction was obsd. for the Cd deriv., Cd-1, which
displays a 1H NMR spectrum identical to that of Zn-2. In attempts to
promote thioether binding, the iodide was displaced by addn. of AgBF4 to
solns. of Zn-2 or the BF4- analog was synthesized directly from Zn(BF4)2
and methylated ligand, Me2bme-daco, to yield Zn-3. Similar reactions with
the Cd analog yielded a product identified as Cd-3 that was
indistinguishable from Zn-3 by 1H NMR. The 113Cd NMR spectra of Cd-3
displayed a single resonance at 88 ppm consistent with a hard donor
environment and inconsistent with S binding. As a further attempt to
induce thioether binding to Zn, the macrocyclization reagent
1,3-dibromopropane was added to Zn-1. The resulting product,
[BrZn(macrocycle)]+, was only slightly sol. in pyridine and identified by
+FAB/MS as the desired macrocyclic product with a large amt. of free

macrocyclic ligand. Recrystn. from pyridine/ether resulted in loss of the Zn as $\text{Zn}(\text{py})_2\text{Br}_2$, which was obtained as colorless crystals and characterized by x-ray crystallog. Complex $\text{Zn}(\text{py})_2\text{Br}_2$ crystallizes in the monoclinic space group $P2_1/c$ with a 8.534(2), b 18.316(4), c 8.461(2) Å, β 101.07(3)°, and $Z = 4$.

RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1998:276384 CAPLUS
DN 129:48710
TI Synthesis and structure of mercury(II) complexes with iminodiacetic, nitrilotriacetic, ethylenediaminetetraacetic, and diethylenetriaminepentaacetic acids
AU Ivanov, S. A.; Martynenko, L. I.; Ilyukhin, A. B.
CS Vysh. Kolledzh Nauk o Mater., MGU, Moscow, Russia
SO Zhurnal Neorganicheskoi Khimii (1998), 43(3), 413-420
CODEN: ZNOKAQ; ISSN: 0044-457X
PB MAIK Nauka
DT Journal
LA Russian
AB $\text{Hg}(\text{IDA}) \cdot 4/3\text{H}_2\text{O}$ (I; H_2IDA = iminodiacetic acid), $\text{Hg}(\text{HNTA})$ (II; H_3NTA = nitrilotriacetic acid), $[\text{Hg}(\text{H}_2\text{L})]_n \cdot n\text{H}_2\text{O}$ (III; H_4L = EDTA) and $\text{K}[\text{Hg}(\text{H}_2\text{DTPA})] \cdot 2\text{H}_2\text{O}$ (IV; H_5DTPA = diethylenetriaminepentaacetic acid) were prepd. and characterized by x-ray structural anal., IR spectra and pH-metric titrns. I, II and III have a framework, chain and framework-type structures, resp. The crystal structure of II was not solved.

L7 ANSWER 3 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1998:270754 CAPLUS
DN 129:4638
TI Formation of 1,11-bis(pendant donor)-cyclam derivatives via the formamidinium salt (cyclam = 1,3,8,11-tetraazacyclotetradecane)
AU Davies, Philip J.; Taylor, Max R.; Wainwright, Kevin R.
CS Dep. Chem., Flinders Univ. South Australia, Adelaide, 5001, Australia
SO Chemical Communications (Cambridge) (1998), (7), 827-828
CODEN: CHCOFS; ISSN: 1359-7345
PB Royal Society of Chemistry
DT Journal
LA English
AB When reacted in chloroform, the di-Me acetal of DMF and cyclam (1,4,8,11-tetraazacyclotetradecane) forms a stable formamidinium salt which can be used as an intermediate for very simple formation of 1,11-bis(pendant donor)-cyclam derivs.

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1997:747600 CAPLUS
DN 128:42925
TI Mixed ligand ethylenediaminetetraacetate cobalt(II), nickel(II), copper(II), and zinc(II) complexes with ammonia and hydrazine
AU Kryatov, S. V.; Budarin, L. I.
CS Inst. Fiz. Khim. im. L. V. Pissarzhevskogo, NAN Ukrainy, Kiev, Ukraine
SO Zhurnal Neorganicheskoi Khimii (1997), 42(4), 610-613
CODEN: ZNOKAQ; ISSN: 0044-457X
PB MAIK Nauka
DT Journal
LA Russian
AB $\text{Na}_2[\text{ML}] \cdot n\text{H}_2\text{O}$ ($M = \text{Co}, \text{Ni}, \text{Cu}, \text{Zn}$; $\text{H}_4\text{L} = \text{EDTA}$) reacted with gaseous NH_3 or $\text{N}_2\text{H}_4 \cdot \text{H}_2\text{O}$ vapors to give $\text{Na}_2[\text{ML}(\text{NH}_3)] \cdot x\text{H}_2\text{O}$ ($M = \text{Co}, \text{Ni}, \text{Cu}, \text{Zn}$) and $\text{Na}_2[\text{ML}(\text{N}_2\text{H}_4)] \cdot y\text{H}_2\text{O}$ ($M = \text{Co}, \text{Ni}, \text{Zn}$), resp. The complexes were characterized by visible absorption and IR spectra. The stepwise

formation consts. were detd. for [MLQ]2- (Q = NH₃, N₂H₄) and [ML(N₂H₄)₂]2- in aq. soln. at 25.degree..

L7 ANSWER 5 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1997:347191 CAPLUS
DN 127:46819
TI Cobalt(III) Polyamine Complexes as Catalysts for the Hydrolysis of Phosphate Esters and of DNA. A Measurable 10 Million-Fold Rate Increase
AU Hettich, Ronald; Schneider, Hans-Joerg
CS FR Organische Chemie der Universitaet des Saarlandes, Saarbruecken, D 66041, Germany
SO Journal of the American Chemical Society (1997), 119(24), 5638-5647
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
AB Complexes between cobalt(III) and eight different 1,4,7,10-tetraazacyclododecane (cyclen) as well as two tris(3-aminopropyl)amine (trpn) derivs. are reported with varying nos. and structures of peralkylammonium groups in side chains of the ligands. The presence of addnl. pos. charges has small effects on hydrolysis rates of nitrophenyl- and bis(nitrophenyl)phosphate esters but leads to substantially enhanced cleavage of plasmid DNA. Increasing the no. of the charged side groups and/or their distance to the metal ion center provides for better binding to the DNA groove, as shown also by affinity measurements with calf-thymus DNA. In line with this, satn. kinetics of plasmid DNA cleavage yield a corresponding increase of efficiency in Michaelis-Menten-type KM values, with rather const. kcat parameters. A binuclear cobalt complex with two cyclen centers sepd. by a -(CH₂)₆-N+(CH₃)₂-(CH₂)₆-N+(CH₃)₂-(CH₂)₆- spacer shows, with only 5.times.10⁻⁵ M catalyst concn., the largest known rate enhancement factor of >10⁷ (corresponding to >10¹¹ at 1 M) against DNA; incubation with 0.05 mM at 37.degree. for only 2 h leads to almost complete cleavage without appearance of products typical for redox cleavage. These results are in contrast to expts. with corresponding copper(II) complexes with added hydrogen peroxide, which has no effect with corresponding Co, Zn, Cd, or Ni complexes.

L7 ANSWER 6 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1997:86118 CAPLUS
DN 126:199780
TI Efficient and unique cooperation of three zinc(II) ions in the hydrolysis of diribonucleotides by a trinuclear zinc(II) complex
AU Yashiro, Morio; Ishikubo, Akira; Komiyama, Makoto
CS Dep. Chem. and Biotech., Sch. Eng., Univ. Tokyo, Tokyo, 113, Japan
SO Chemical Communications (Cambridge) (1997), (1), 83-84
CODEN: CHCOFS; ISSN: 1359-7345
PB Royal Society of Chemistry
DT Journal
LA English
AB A trinuclear Zn₂⁺ complex is prepd. using a ligand having six pyridine moieties, N,N,N',N',N'',N''-hexakis(2-pyridylmethyl) [tris(2-aminoethyl)amine] (L3), and efficiently hydrolyses diribonucleotides at pH 7 and 50.degree., showing much greater activity than a dinuclear Zn₂L₂ complex.

RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 7 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1996:752767 CAPLUS
DN 126:150683
TI Synthesis and properties of zinc-nitrogen compounds for the MOVPE of p-type ZnSe
AU Pohl, U. W.; Freitag, S.; Gottfriedsen, J.; Richter, W.; Schumann, H.

CS Technische Universitaet Berlin, Institut fuer Festkoerperphysik, Sekr. PN
6-1, Hardenbergstrasse 36, Berlin, D-10623, Germany
SO Journal of Crystal Growth (1997), 170(1-4), 144-148
CODEN: JCRGAE; ISSN: 0022-0248
PB Elsevier
DT Journal
LA English
AB Novel N-based compds. for p-type doping of ZnSe have been studied.
Photoluminescence spectra of epilayers doped with synthesized Zn amides
Zn(NRR')₂ and with corresponding amines HNRR' (R and R' are org. ligands)
indicate an insufficient stability of the Zn-N bond, preventing effective
doping of the tested Zn amides. Doping efficiency is improved by
replacing tert-Bu groups (-CMe₃) of the ligands by trimethylsilyl groups
(-SiMe₃). N incorporation under usual growth conditions remained,
however, too low for device applications.
RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 8 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1996:720938 CAPLUS
DN 126:54072
TI The coordination ability of N,N'-ethylenebis(2-amino 1-butanol)
dihydrochloride towards transition and representative metals
AU Ali, Taj; Rehman, Obaidur; Ali Khan, Shad; Rauf, A.
CS Department Chemistry, Univ. Peshawar, Pak.
SO Journal of the Chemical Society of Pakistan (1996), 18(3),
191-196
CODEN: JCSPDF; ISSN: 0253-5106
PB Chemical Society of Pakistan
DT Journal
LA English
AB N,N'-Ethylenebis(2-amino 1-butanol) dihydrochloride (EBAB) reacts with
divalent transition metal salts to give MLX₂ where L = EBAB, M = Cu, Ni,
Co, Cd and Hg; X = Cl, Br, NO₃. These complexes were characterized by
elemental anal., cond. measurements, room temp. magnetic moment studies,
electronic and IR spectra. The ligand in these complexes behaves as
bidentate like substituted ethylenediamine coordinating through N atoms.
The solid state IR study and other data support distorted tetrahedral
geometry MN₂X₂.

L7 ANSWER 9 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1996:710375 CAPLUS
DN 126:41814
TI A Novel Biomimetic Zinc(II)-Fluorophore, Dansylamidoethyl-Pendant
Macrocyclic Tetraamine 1,4,7,10-Tetraazacyclododecane (Cyclen)
AU Koike, Tohru; Watanabe, Tomohiko; Aoki, Shin; Kimura, Eiichi; Shiro, Motoo
CS School of Medicine, Hiroshima University, Hiroshima, 734, Japan
SO Journal of the American Chemical Society (1996), 118(50),
12696-12703
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
AB From the chem. principle of carbonic anhydrase (CA)-arom. sulfonamide
inhibitor interaction, a dansylamidoethyl-pendant cyclen
(1-(2-(5-(dimethylamino)-1-naphthalenesulfonamido)ethyl)-1,4,7,10-
tetrazacyclododecane, HL) was synthesized as a novel type of
Zn(II)-fluorophore. The new ligand HL forms very stable complexes (ML)
with Zn(II), Cd(II), and Cu(II) at physiol. pH. The potentiometric and
spectrophotometric pH-titrn. study disclosed the 1:1 metal(II) complexes
stability consts. log K(ML) (= log([ML]/[M][L])) to be 20.8 +/- 0.1 for
ZnL, 19.1 +/- 0.1 for CdL, and >30 for CuL. The cryst. Zn(II) complex
ZnL was isolated from aq. soln. at pH 7. The x-ray crystal study of ZnL
disclosed a five-coordinate, distorted square-pyramidal structure with the

deprotonated dansylamide N- coordinating at the apical site. Crystals of the monoperchlorate salt of ZnL (C₂₂H₃₅N₆O₆SClZn) are orthorhombic, space group Pna2₁ with a 23.777(3), b 12.744(5), c 9.092(3) .ANG., Z = 4, R = 0.032, and Rw = 0.047. The Zn(II) complex shows a max. UV absorption band (.lambda.max) at 323 nm (.epsilon. 5360) at 25.degree. in aq. soln. The fluorescent max. and the quantum yield (.PHI.) of ZnL vary with the solvent: at 528 nm (.PHI. = 0.11) in H₂O, 496 nm (0.53) in MeOH, 489 nm (0.60) in EtOH, and 484 nm (0.44) in MeCN. Demetalation of ZnL with excess amt. of EDTA yielded the metal-free ligand HL, which in pH 7.3 aq. soln. has an excitation and a weak emission fluorescence at 330 nm (.epsilon. 4950) and 555 nm (.PHI. = 0.03), resp. The Cu(II) ion, to the contrary, completely quenches the fluorescence. The cryst. Cu(II) complex CuL (.lambda.max 306 nm, .epsilon. 7630 in H₂O) was isolated as its monoperchlorate salt. The Zn(II)-dependent fluorescence with 5 .mu.M HL at pH 7.3 is quant. responsive to 0.1-5 .mu.M concn. of Zn(II), which is unaffected by the presence of mM concn. of biol. important metal ions such as Na⁺, K⁺, Ca²⁺, and Mg²⁺. The new ligand HL forms a far more stable 1:1 Zn(II) complex than any previous Zn(II) fluorophore and is evaluated as a new Zn(II) fluorophore.

- L7 ANSWER 10 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1996:683864 CAPLUS
 DN 125:320798
 TI Trinuclear Zn(II) complex for the efficient and structure dependent hydrolysis of RNA
 AU Yashiro, Morio; Ishikubo, Akira; Komiyama, Makoto
 CS Dep. Chem. Biotechnol., Univ. Tokyo, Tokyo, 113, Japan
 SO Nucleic Acids Symposium Series (1996), 35 (Twentythird Symposium on Nucleic Acids Chemistry, 1996), 103-104
 CODEN: NACSD8; ISSN: 0261-3166
 PB Oxford University Press
 DT Journal
 LA English
 AB A trinuclear Zn(II) complex is newly prepd. using a ligand having six pyridine moieties, N,N,N',N',N'',N''-hexakis(2-pyridylmethyl){tris-(2-aminoethyl)amine} (L1). The trinuclear Zn(II)3-L1 complex efficiently hydrolyzes diribonucleotides at pH 7 and 50 .degree.C; its activity is much greater than that of a dinuclear (Zn(II))2-(1,3-bis[bis(2-pyridinylmethyl)amino]-2-propanol) complex. The hydrolysis by the trinuclear Zn(II)3-L1 complex is also unique in the product ratio; highly selective over the 2'-monophosphate is obsd.
- L7 ANSWER 11 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1996:165336 CAPLUS
 DN 124:276900
 TI Synthesis of mixed-ligand complexes of aminopolycarboxylates of 3d-metals with ammonia and hydrazine
 AU Kryatov, S. V.; Budarin, L. I.
 CS Inst. Fiz. Khim. im. Pisarzhevskogo, Kiev, Ukraine
 SO Dopovidi Natsional'noi Akademii Nauk Ukraini (1995), (9), 87-9
 CODEN: DNAUFL
 PB Naukova Dumka
 DT Journal
 LA Russian
 AB Nitritotriacetates NaMNTA.cntdot.H2O and ethylenediaminetetraacetates Na2MEDTA.cntdot.(3-4)H2O (M = Co, Ni, Cu, Zn) react reversibly with NH₃ in the presence of water vapor and N₂H₄.cntdot.water vapor, forming mixed-ligand amino-complexes Na[MNTA(NH₃)(OH₂)] .cntdot.3H₂O and Na2[MEDTA(NH₃)] .cntdot.(5-6)H₂O (M = Co, Ni, Cu, Zn) and hydrazine complexes Na[MNTA(N₂H₄)₂] .cntdot.2H₂O (M = Co, Ni, Zn) and Na2[MEDTA(N₂H₄)] .cntdot.(5-6)H₂O. The aminopolycarboxylates of Cu(II) are reduced with N₂H₄ to metal. The coordination structures of the complexes were assigned from their visible and IR-spectra.

L7 ANSWER 12 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1995:870966 CAPLUS
 DN 123:298334
 TI Thermal decomposition kinetics of Co(II), Ni(II), Cu(II) and Zn(II) complexes of dihydrazinium ethylenediamine-tetraacetate
 AU Saravanan, N.; Yusuff, K. K. Mohammed
 CS Dep. Applied Chem., Cochin Univ. Sci. Technol., Cochin, 682 022, India
 SO Reaction Kinetics and Catalysis Letters (1995), 55(2), 407-14
 CODEN: RKCLAU; ISSN: 0304-4122
 PB Akademiai Kiado
 DT Journal
 LA English
 AB Hydrazinium ethylenediaminetetraacetatometalate complexes of the type, $N_2H_5[M(Hedta).H_2O]$ were subjected to systematic TG/DTG anal. The decompn. process consists of three stages. Kinetic parameters were evaluated for each of these stages using the Coats-Redfern equation.

L7 ANSWER 13 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1995:837204 CAPLUS
 DN 123:328244
 TI NMR study of Zn_2TTHA and other complexes with TTHA
 AU Song, Rui-Fang; Mao, You-Gang; Li, Fei; Qin, Song-Yan
 CS Inst. of Theoretical Chem., Jilin Univ., Changchun, 130023, Peop. Rep. China
 SO Gaodeng Xuexiao Huaxue Xuebao (1995), 16(9), 1436-9
 CODEN: KTHPDM; ISSN: 0251-0790
 PB Gaodeng Jiaoyu Chubanshe
 DT Journal
 LA Chinese
 AB The dynamic NMR study of Zn, Mg, Pb and Hg binuclear complexes with TTHA (triethylene-tetraaminhexaacetic acid) is reported. The intramol. rearrangement of Zn_2TTHA is obsd. in the range of the temp. studied and the rate consts. of the rearrangement process are calcd. by the simulating to the exptl. spectra. Probably the structural units of Zn_2TTHA are two octahedral units but not two tetrahedral ones; the activation energies E_a of the binuclear complexes of Mg, Pb and Hg with TTHA are estd. by the Bloch equation of the two sites exchange; and the order of E_a is linearly related to the ion potential of the metal ions.

L7 ANSWER 14 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1995:714472 CAPLUS
 DN 123:245145
 TI Phosphodiester Hydrolysis by a New Zinc(II) Macrocyclic Tetraamine Complex with an Alcohol Pendant: Elucidation of the Roles of Ser-102 and Zinc(II) in Alkaline Phosphatase
 AU Kimura, Eiichi; Kodama, Yorimitsu; Koike, Tohru; Shiro, Motoo
 CS School of Medicine, Hiroshima University, Hiroshima, 734, Japan
 SO Journal of the American Chemical Society (1995), 117(32), 8304-11
 CODEN: JACSAT; ISSN: 0002-7863
 PB American Chemical Society
 DT Journal
 LA English
 AB A new benzyl alc.-pendant 1,4,7,10-tetraazacyclododecane (cyclen) ligand, (S)-1-(2-hydroxy-2-phenylethyl)-1,4,7,10-tetraazacyclododecane (L) (11), was synthesized. The complexation of 11 with Zn^{II} yielded 1:1 five-coordinate complexes (isolated as its perchlorate salts with the pendant alc. either undissociated (ZnL , 14a) or dissocd. ($ZnH-1L$, 14b) from acidic (pH 6.0) or basic (pH 9.5) aq. soln., resp.). The pK_a value for the pendant alc. (14a \rightarrow 14b + H^+) was detd. by potentiometric pH titrn. to be 7.30 \pm 0.02 at 35.degree. with $I = 0.10$ ($NaNO_3$). The x-ray crystal study of 14b showed two crystallog. distinct structures with the alkoxide closely coordinated at the 5th coordination site, where an av. distance of Zn-O- is 1.91 .ANG.. Crystals of 14b.cntdot.ClO4 are

orthorhombic, space group P212121 with a 16.977(4), b 18.135(4), c 13.173(3) .ANG., Z = 8, R = 0.050, and Rw = 0.077. The ZnII-bound alkoxide anion in 14b is a more reactive nucleophile than N-methylcyclen-ZnII-OH- species 15b. In the kinetic study using 14 in aq. soln. (pH 6.0-10.3) at 35.degree. with I = 0.10 (NaNO3), the rate-pH profile for a phosphoryl transfer reaction from bis(4-nitrophenyl) phosphate (BNP-) to 14b gave a sigmoidal curve with an inflection point at pH 7.4, which corresponds to the pKa value for 14a .dblharw. 14b + H+. The 2nd-order rate const. kBNP is 125 times greater than the corresponding value for BNP- hydrolysis catalyzed by 15b. The product of the phosphoryl transfer reaction from BNP- to 14b is the pendant alc.-phosphorylated 16, which was isolated as its perchlorate salt 16a by reacting 14b with BNP- in DMF. In anhyd. DMF soln., the phosphoryl transfer (kBNP of 1.1 .+- . 0.1M-1 s-1 at 35.degree.) is 1700 times faster than that in aq. soln. In the subsequent reaction of 16, the pendant phosphodiester undergoes an intramol. nucleophilic attack by the ZnII-bound OH- of 16b to yield a phosphomonoester product 17. From the sigmoidal rate-pH relation (pH 7.4-10.5), the kinetic pKa value of 9.0 was estd. for 16a .dblharw. 16b + H+, which is almost the same value (pKa = 9.10 .+- . 0.05) detd. by potentiometric pH titrn. at 35.degree.. The 1st-order rate const. for the reaction 16b .fwdarw. 17 is (3.5 .+- . 0.1) .times. 10-5 s-1 at 35.degree. with I = 0.10 (NaNO3). As a ref. to this intramol. phosphodiester hydrolysis, Et (4-nitrophenyl) phosphate (NEP-) was hydrolyzed by 15b. The intramol. hydrolysis is 45,000 times faster than the intermol. NEP- hydrolysis with 1 mM 15b. The present findings that demonstrate the potential of the proximate alc. by ZnII in the initial phosphoryl transfer and the potential of the ZnII-bound H2O in the intramol. phosphate hydrolysis may well serve to elucidate the collaborative functions of Ser-102 and ZnII ions in alk. phosphatase.

L7 ANSWER 15 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1995:608216 CAPLUS

DN 123:101267

TI The Amide Oxygen as a Donor Group. Metal Ion Complexing Properties of Tetra-N-acetamide Substituted Cyclen: A Crystallographic, NMR, Molecular Mechanics, and Thermodynamic Study

AU Maumela, Hulisani; Hancock, Robert D.; Carlton, Laurence; Reibenspies, Joseph H.; Wainwright, Kevin P.

CS Department of Chemistry, University of the Witwatersrand, Johannesburg, 2050, S. Afr.

SO Journal of the American Chemical Society (1995), 117(25), 6698-707

CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English

AB The syntheses of the octadentate ligand DOTAM (1,4,7,10-tetrakis(acetamido)-1,4,7,10-tetraazacyclododecane) and its complexes with Zn(II), Cd(II), and Ca(II) are described. Crystal structures of [Cd(DOTAM)](ClO4)2.cntdot.1.5H2O (1), [Ca(DOTAM)](ClO4)2.cntdot.2.5H2O (2), and [Zn(DOTAM)](ClO4)2.cntdot.H2O (3) are reported. Crystal data: (1) monoclinic, space group Cc, a 11.908(2), b 21.237(3), c 11.445(2) .ANG., .beta. 102.15(1).degree.; (2) monoclinic, P21/c, a 14.031(9), b 11.469(8), c 17.448 .ANG., .beta. 92.10(1).degree.; (3) triclinic, space group P.hivin.1, a 9.490(1), b 12.464(2), c 12.998(2) .ANG., .alpha. 99.070(1), .beta. 107.67(1), and .gamma. 108.24(1).degree.. There is an unusual distortion in the coordination geometry of the complexes. There are two sets of metal-to-O bond lengths for each complex; Zn(II) has two oxygens, placed opposite each other in the approx. square arrangement defined by the four O donor atoms at .apprx.2.19 .ANG. and two at 3.23 .ANG., Cd(II) has two at 2.34 and two at 2.64 .ANG., and Ca(II) has two at 2.40 .ANG. and two at 2.42 .ANG.. Mol. mechanics calcns. suggest the Cd(II) and Zn(II) structures represent six coordination of four nitrogens and two of the oxygens, while the two long bonds represent van der Waals

contacts with a possible electrostatic component. Approach of the O donors to the metal ion is controlled by the van der Waals radii of the oxygens. ¹³C NMR studies give rates of helicity interchange of the complexes Zn(II) > Hg(II) > Cd(II) > Ca(II) .mchgt. Pb(II). This order is discussed in terms of the difference in bond lengths between the two sets of O donors. A stability const. study gave logK₁ values in 0.1M NaNO₃ and 25.degree.: Cu(II), 16.3; Zn(II), 10.47; Ca(II), 7.54; Sr(II), 6.67; Ba(II), 5.35; Hg(II), 14.53; La(III), 10.35; Gd(III), 10.05. For Cd(II) and Pb(II), the complexes were fully formed even at pH 0.3, and only a lower limit of 19 for logK₁ could be set. Selectivity of DOTAM for metal ions is discussed in terms of coordinating properties of the amide O donor and geometric requirements of the DOTAM ligand.

L7 ANSWER 16 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1995:481834 CAPLUS
 DN 122:284776
 TI Efficient Cleavage of DNA by Iron(III) Triazacyclononane Derivatives
 AU Silver, Gail C.; Trogler, William C.
 CS Department of Chemistry, University of California, San Diego, La Jolla, CA, 92093-0358, USA
 SO Journal of the American Chemical Society (1995), 117(14), 3983-93
 CODEN: JACSAT; ISSN: 0002-7863
 PB American Chemical Society
 DT Journal
 LA English
 AB Compsd. based on (1,4,7-trimethyl-1,4,7-triazacyclononane)iron(III) chloride have been synthesized. Exceedingly low concns. (approx. 0.5 .mu.M) of these reagents are required to effect single-stranded oxidative cleavage of plasmid DNA at physiol. pH and temp. Approx. 3 breaks per plasmid per micromolar of reagent occur in 1 h at 37.degree.. The addn. of dithiothreitol dramatically increased the effectiveness of these compds.; only 0.05 .mu.M of reagent was required for DNA cleavage. When psoralen (a DNA photo-crosslinking agent) was attached to the iron complex, irradiation further increased the cleavage efficiency. The DNA cleaving abilities rival those of the cytotoxic antitumor drug bleomycin. Unlike bleomycin, the synthetic agents cut DNA with little sequence specificity. The lability of the chloride ligands, the hard acid character of iron(III), and the absence of base specificity in the DNA cleaving reaction suggest that a cationic iron species binds to the phosphate backbone of DNA. The reaction's dependence on reductants and dissolved oxygen suggests that it proceeds by a redox mechanism. Crystals of (1,4,7-trimethyl-1,4,7-triazacyclononane)FeCl₃ (L'FeCl₃) belong to the monoclinic space group P2₁/c, with a = 12.321(2) .ANG., b = 7.3220(10) .ANG., c = 15.903(3) .ANG., V = 1434.7(5) .ANG.³, and Z = 4 at 293 K. Refinement of 145 least squares parameters for 2613 independent reflections with F > 4.0.sigma.(F) converged to R = 3.43% and Rw = 6.45%. The coordination geometry around iron(III) approximates a trigonally distorted octahedron. The N-Fe-N bond angles (77.8.degree.-78.8.degree.) are compressed, while the Cl-Fe-Cl angles (96.7.degree.-97.0.degree.) are expanded from the octahedral value.

L7 ANSWER 17 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1995:481676 CAPLUS
 DN 122:229225
 TI Zinc Complexes of the Ligand Dipicolylglycine
 AU Abufarag, Ahmed; Vahrenkamp, Heinrich
 CS Institut fuer Anorganische und Analytische Chemie, Universitaet Freiburg, Freiburg, D-79104, Germany
 SO Inorganic Chemistry (1995), 34(8), 2207-16
 CODEN: INOCAJ; ISSN: 0020-1669
 PB American Chemical Society
 DT Journal
 LA English

AB N,N-bis(2-picoly)glycine (L-H) which was not obtained in the free state was introduced into Zn complexes via its Et ester (L-Et) which yielded the intermediate complexes (L-Et)ZnBr₂ (1), (L-Et)Zn(NO₃)₂ (2), and (L-Et)₂Zn(ClO₄)₂.cntdot.H₂O (3). Autocatalytic hydrolysis in the presence of H₂O turned 2 into [L.cntdot.Zn(H₂O)₂]NO₃.cntdot.H₂O (4) with an octahedral and 3 into trimeric [L.cntdot.Zn]ClO₄.cntdot.H₂O (5) with a trigonal-bipyramidal coordination of Zn in the solid state. 5 is a good starting material for the introduction of coligands forming complexes that mimic the coordination of Zn in enzymes with a N,N,O donor set: with imidazole the octahedral complex [L.cntdot.Zn(Im)(H₂O)]ClO₄ (6) was obtained, with 2-methylimidazole the trigonal-bipyramidal complex [L.cntdot.Zn(MeIm)]ClO₄ (7), and with di-Ph phosphate the trigonal-bipyramidal complex [L.cntdot.Zn(Phos)].cntdot.2H₂O (8). The coordination in the solid state was confirmed for 1 and 4-8 by x-ray work. NMR studies (solid state and soln.) and cond. measurements revealed various states of dissocn. and solvation in soln., with the trigonal-bipyramidal cation [L.cntdot.Zn(H₂O)]⁺ probably being a common and major constituent of all aq. equil.

L7 ANSWER 18 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1995:319991 CAPLUS

DN 122:234214

TI The catalytic carboxyester hydrolysis by a new zinc(II) complex with an alcohol-pendant cyclen (1-(2-hydroxyethyl)-1,4,7,10-tetraazacyclododecane): A novel model for indirect activation of the serine nucleophile by zinc(II) in zinc enzymes

AU Koike, Tohru; Kajitani, Satoko; Nakamura, Ikushi; Kimura, Eiichi; Shiro, Motoo

CS School of Medicine, Hiroshima University, Hiroshima, 734, Japan

SO Journal of the American Chemical Society (1995), 117(4), 1210-19

CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

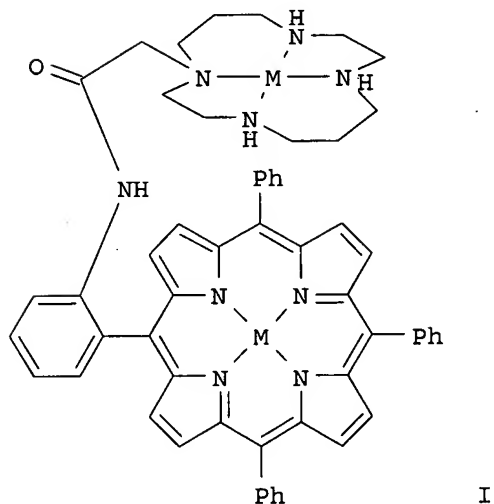
DT Journal

LA English

AB A new macrocyclic tetraamine (cyclen) having a strategically appended alc. group, 1-(2-hydroxyethyl)-1,4,7,10-tetraazacyclododecane, was synthesized. The functionalized cyclen formed a 1:1 ZnL complex (I) at pH .apprx.6. An x-ray crystal structure study disclosed a 5-coordinate structure with the undeprotonated alc. OH group coordinating at an apical position. Crystals of I.cntdot.(ClO₄)₂ (C₁₀H₂₄N₄O₉Cl₂Zn) were monoclinic, space group P2₁/n with a = 8.813, b = 23.662, c = 8.814 .ANG., .beta. = 90.21.degree., V = 1838.0 .ANG.³, Z = 4, R = 0.073, and Rw = 0.125. Potentiometric pH titrn. of I showed the dissocn. of a proton with a pK_a of 7.60 at 25.degree. and I = 0.10 (NaClO₄). From NMR and competitive anion-binding studies, the structure of the deprotonated species was assigned to be a OH--bound ZnL-OH- complex (II). During unsuccessful attempts to isolate the deprotonated species, the authors obtained a trimeric phosphate complex, (ZnL-O-)₃P:O, as its PF₆- salt (III.cntdot.(PF₆)₃(H₂O)_{1.5}) from pH 9.5 aq. soln. contg. I.cntdot.(ClO₄)₂, K₂HPO₄, and NH₄PF₆. Crystals of III.cntdot.(PF₆)₃(H₂O)_{1.5} (detd. as the trimer of C₁₀H₂₅N₄O₁₇/6P₄/3F₆Zn) were trigonal, space group R₃, with a = 23.353, c = 17.527 .ANG., V = 8278 .ANG.³, Z = 18, R = 0.070, and Rw = 0.112. Among the known ZnII complexes, ZnL-OH- complex II was the most active catalyst for 4-nitrophenyl acetate (NA) hydrolysis. In the kinetic studies using I in 10% CH₃CN at 25.degree., I = 0.10 (NaNO₃), and pH 6.4-9.5, the pH-rate profile gave a sigmoidal curve with an inflection point at pH 7.7, which corresponded to a pK_a for I (ZnL) .dblharw. II (ZnL-OH-) + H⁺. The 2nd-order (1st-order each in [II] and [NA]) rate const. of 0.46 M⁻¹ s⁻¹ was .apprx.10-fold greater than the corresponding value of 4.7 .times. 10⁻² M⁻¹ s⁻¹ for the N-methylcyclen-ZnII-OH- complex catalyst. Furthermore, it was found that NA hydrolysis occurred through a double-displacement reaction of the acetyl group. In the 1st rate-detg. reaction, the nucleophile was the pendant alc. OH group activated by the adjacent ZnII-OH-, which attacked NA to yield an acyl intermediate (IV).

This intermediate was independently synthesized by the reaction of I with acetic anhydride in CH₃CN. In the 2nd reaction, IV was subject to extremely fast hydrolysis (e.g., $t_{1/2}$ = 6 s at pH 9.3), as monitored on spectral change of pH-indicators. A plot of the obsd. 1st-order rate consts. against pH (6.1-9.3) for the 2nd process gave a sigmoidal curve with its inflection point at pH 7.7, which was similar to the pK_a values of 2 ZnII-cyclen complexes. It was concluded that the very fast 2nd reaction occurs through the nucleophilic attack of the ZnII-OH⁻ at the intramol. acetyl group of IV. The overall NA hydrolysis by II was catalytic. Thus, the OH⁻-bound ZnL plays dual roles: as a general base in the 1st acyl-transfer reaction to activate the remote alc. OH and as a nucleophile to attack the electrophilic center in the 2nd hydrolysis step. Such a dyad of ZnII-OH⁻ and the adjacent alc. OH may account for the strong nucleophilicity of Ser at the active center of Zn enzymes such as alk. phosphatase.

L7 ANSWER 19 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1994:644100 CAPLUS
 DN 121:244100
 TI Synthesis of novel heterobimacrocyclic complexes based on porphyrin and cyclam. Study of their reactivity toward dioxygen
 AU Koeller, S.; Cocolios, P.; Guillard, R.
 CS Lab. Ing. Mol. Separation App., Faculte des Sciences "Gabriel", Dijon, 21000, Fr.
 SO New Journal of Chemistry (1994), 18(7), 849-59
 CODEN: NJCHE5; ISSN: 1144-0546
 DT Journal
 LA French
 GI



AB A new Porphyrin-Cyclam dinucleating ligand was prepd. The authors report here its synthesis and several homo- and heterobimetallic derivs. (e.g. I(OAc)₂; M = Zn, Cu, Co; M' = Zn, Cu, Co). Some results unambiguously show that the 2 macrocycles can adopt a face to face geometry but no definitive conclusion can be made concerning the conformation of the bimetallic complexes. The authors also discuss the reactivity of the Co-contg. complexes towards dioxygen, and the authors report the 1st example of .mu.-peroxo intermol. complexes in org. solvents.

L7 ANSWER 20 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1994:498394 CAPLUS
 DN 121:98394
 TI Reaction of dihydrazinium ethylenediaminetetraacetate with nitrates of Co(II), Ni(II), Cu(II) and Zn(II)
 AU Saravanan, N.; Sivasankar, B. N.; Govindarajan, S.; Yusuff, K. K. Mohammed
 CS Dep. Chem., Bharathiar Univ., Coimbatore, 641 046, India
 SO Synthesis and Reactivity in Inorganic and Metal-Organic Chemistry (1994), 24(5), 703-13
 CODEN: SRIMCN; ISSN: 0094-5714
 DT Journal
 LA English
 AB The dihydrazinium ethylenediaminetetraacetate, (N₂H₅)₂(H₂EDTA) reacts with metal nitrates to form N₂H₅[M(Hedta).H₂O] (M = Co, Ni, Cu or Zn). These complexes were characterized by anal. data, cond. and magnetic susceptibility measurements, electronic and IR spectroscopy and thermal analyses. The complexes are 1:1 electrolytes in aq. soln.

L7 ANSWER 21 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1994:456525 CAPLUS
 DN 121:56525
 TI Plant response to foliar application of essential trace metal complexonates.
 AU Bitiutsky, N. P.; Kaschenko, A. S.
 CS Biol. Nauchno-Issled. Inst., St. Peterburg. Gos. Univ., Russia
 SO Agrokhimiya (1992), (5), 102-9
 CODEN: AGKYAU; ISSN: 0002-1881
 DT Journal
 LA Russian
 AB Mn deficiency depressed chlorophyll and growth in hydroponic cucumbers. Zn deficiency depressed the growth only. Spraying 1.8.10-3M MnSO₄ and Mn diethylenetriamine-N,N,N',N'',N'''-pentaacetate equally effectively restored chlorophyll and growth, whereas Mn 1-hydroxyethylidenediphosphonate caused Mn chlorosis and severely suppressed growth. Spraying 1.8.10-3M ZnSO₄ and Zn diethylenetriamine-N,N,N',N'',N'''-pentaacetate equally effectively restored growth. Spraying Mn, Zn and Cu complexonates stimulated the growth of potted annual ryegrass by 7-12%. ZnSO₄ increased, whereas CoSO₄ decreased by 20%, foliar chlorophyll on limed soil. MnSO₄ and CuSO₄, but not the complexonates, transiently inhibited nitrate reductase in young ryegrass plants. Zn, Cu, and Co sulfates decreased ryegrass protein content. Zn and Cu sprays strongly, whereas Mn slightly, decreased ryegrass Mn concn. Zn decreased plant Cu and the sulfates of all the trace metals besides Co decreased plant Co. Foliar sprays with ZnSO₄ or Cu diethylenetriamine-N,N,N',N'',N'''-pentaacetate increased barley grain yield from 26.7 to 30.2 and 29.2 g/pot, resp. Other treatments were ineffective or showed a low effectiveness. Only ZnSO₄ increased the protein yield/pot in barley grain. Cu and Co sprays decreased grain Mn and Cu, resp. In general, sulfates were more effective than complexonates.

L7 ANSWER 22 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1994:259804 CAPLUS
 DN 120:259804
 TI Formation of cadmium(II) nitrate complexes with macrocycles
 AU Kim, Ho Doo; Jung, Hak Jin; Jung, Oh Jin
 CS Koryo Cement Co., Jang-Sung, 515-800, S. Korea
 SO Bulletin of the Korean Chemical Society (1993), 14(5), 561-7
 CODEN: BKCSDE; ISSN: 0253-2964
 DT Journal
 LA English
 AB Twelve macrocycle (L) complexes of Cd(II) nitrate were synthesized: CdL(NO₃)₂. All the complexes were identified by elemental anal., elec. cond. measurements, IR and NMR spectroscopic techniques. The molar elec. conductivities of the complexes in H₂O and MeCN solvent were at 236.8-296.1 cm² mol⁻¹ .OMEGA.-1 at 25.degree.. The characteristic peaks

of macrocycles affected by Cd(II) were shifted to lower frequencies as compared with uncomplexed macrocycles. A complex with 1,4,8,11-tetraazacyclotetradecane-1,4,8,11-tetraacetic acid (L4) exhibited 2 characteristic bands such as strong stretching (1646 cm⁻¹), and weaker sym. stretching band (1384 cm⁻¹). NMR studies indicated that all N donor atoms of macrocycles have greater affinity to Cd(II) metal ion than do the O atoms. The ¹³C-resonance lines of methylene groups neighboring the donor atom such as N and S were shifted to a direction of high magnetic field and the order of chem. shifts were L1<L2<L3<L6<L4. Also the chem. shifts values were larger than those of methylene groups bridgeheaded in side-armed groups. This result seems due to not only the strong interaction of Cd(II) with N donors according to the HSAB theory, but weak interaction of Cd(II) and COO⁻ ions or S which is enhanced by the flexible methylene spacing group in side-armed groups. Thus, each addnl. geminal-Me pairs of L3, L4 and L6 macrocycles relative to L1, L2, and L5 leads to an large enhancement in Cd(II) affinity. ¹³C-NMR spectrum of the complex with L12 (1,5,9,13-tetrathiacyclohexadecane-3,11-diol) reveals 2 sets of 3 resonance lines, and intensities of the each resonance line have the ratio of 1:2:2. This mol. conformation is predicted as structure of tetragonal complex to be formed by coordinating 2 S atoms and the other 2 S atoms which is affected by OH-groups.

L7 ANSWER 23 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1993:255902 CAPLUS

DN 118:255902

TI Structure of the epoxy-chelate metal-containing matrices: theoretical aspects

AU Kurnoskin, A. V.

CS Sci. Prod. Unit, "Stekloplastik", Kryukovo, Russia

SO Journal of Applied Polymer Science (1993), 48(4), 639-56

CODEN: JAPNAB; ISSN: 0021-8995

DT Journal

LA English

AB A theor. anal. was carried for the structural anal. of metalliferous epoxy-chelate polymers (MECP) based on diglycidyl ether of bisphenol A (DGEBA) hardened with metal complexes of the formula [M(L)_n(X)_p], where M is the cation of the transition metal; R is a N-contg. ligand; X is the anion of an org. acid; n is the no. of the ligands in the complex mol. (n = 1 or 2), and p is the metal valency (p = 2 or 3). On the basis of the correlations between the tensile strength (.sigma.t) and tensile modulus (Et), and flexural strength (.sigma.f) and flexural modulus (Ef) of MECP, .sigma.t = f(Et) and .sigma.f = f(Ef), and supposing that when the condition .sigma.tA = .sigma.tB, .sigma.fA = .sigma.fB, EtA = EtB, EfA = EfB is fulfilled, where A and B are complex hardeners of different structures but of the same class, the epoxy-chelate matrixes have similar structures. The effect of the structural fragments on the hardener mol. (the metal, ligand, and anion) on the polymer properties was evaluated and it was found out that the biggest contribution of these properties belongs to the metal, the alteration of which changes the thermal stability (.DELTA.M), deformability (.epsilon.), .sigma.f, Ef, and deflection temp. (DT) significantly. By this, the effect of the hardener structure change on the alteration of the MECP properties is maximal for .DELTA.M, is minimal for the compressive strength (.sigma.c), and decreased in the series: .DELTA.M > .epsilon. > DT > .sigma.f > Ef > .sigma.c. The type of the anion affects .sigma.c significantly, but the ligand type contributes the least to the polymer properties.

L7 ANSWER 24 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1993:199215 CAPLUS

DN 118:199215

TI The mechanism of the intramolecular rearrangement of HEDTA metal complexes - the dynamic NMR study

AU Song, Ruifang; Li, Fei; Li, Liang

CS Inst. Theor. Chem., Jilin Univ., Changchun, 130023, Peop. Rep. China

SO Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy (1993), 49A(2), 285-9
 CODEN: SAMCAS; ISSN: 0584-8539
 DT Journal
 LA English
 AB The ¹H NMR spectra of the complexes of K, Mg, Ca, Sr, Ba, and Zn ions with N-hydroxyethylethylenediaminetriacetic acid (HEDTA) were measured at various temps. The chem. shifts of the protons on acetates and the backbone change with temp., while those of the hydroxyethylenic protons do not, and the AB quartet arising from the single acetate coalesces into a singlet with the increase of temp. The mechanism of the intramol. rearrangement is given in which the .DELTA., .LAMBDA. conversion and nitrogen inversion occur almost in the same time. The stability of these metal complexes decreases in the order Zn > alk. earth metal > K, which is in agreement with the order of the ionic potential of the central ions. Activation energies are given for the Zn complex.

L7 ANSWER 25 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1992:596520 CAPLUS
 DN 117:196520
 TI Sand molds and cores manufactured using phenolic binder hardened with an ester
 IN Yoshida, Akira; Kyochika, Naoki; Tanaka, Tsutomu; Matsuyama, Katsumi; Kiuchi, Kazuhiko
 PA Kao Corp., Japan
 SO Eur. Pat. Appl., 31 pp.
 CODEN: EPXXDW
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 465919	A1	19920115	EP 1991-110454	19910625 <--
	EP 465919	B1	19980909		
	R: DE, FR, GB				
	JP 04339537	A2	19921126	JP 1991-162943	19910703 <--
	JP 2504638	B2	19960605		
	US 5602192	A	19970211	US 1993-154726	19931119 <--
PRAI	JP 1990-178634		19900705		
	JP 1990-229718		19900831		
	JP 1990-408225		19901227		
	US 1991-719632		19910624		

AB The self-hardening sand binders based on water-sol. phenolic resin contain an org. ester hardener and Group IB-VIII metals and/or compds. (esp., powd. Mg, Zn, salts, oxides, and/or chelate compds.), optionally with organosilane coupling agent. The foundry molds and cores are hardened without heating, show improved strength, and are optionally manufd. from reclaimed foundry sand. Thus, the molded test specimens were manufd. from the mixt. contg. reclaimed SiO₂ sand 100, aq. 49% phenolic resin binder 1.5, and triacetin hardener and additive 0.375 wt. parts each. Compressive strength in 24 h at 25.degree. and 60% relative humidity was 21.2 kg/cm² when the additive was CaCl₂ or 15.5 kg/cm² with Ca(OH)₂, vs. only 4.5 kg/cm² without the additive.

L7 ANSWER 26 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1992:592893 CAPLUS
 DN 117:192893
 TI Application of metalliferous epoxy chelate polymers for composite production
 AU Kurnoskin, A. V.
 CS Sci. Prod. Unit, "Stekloplastik", Kryukovo, Russia
 SO Journal of Macromolecular Science, Pure and Applied Chemistry (1992), A29(12), 1155-73
 CODEN: JSPCE6; ISSN: 1060-1325

DT Journal
LA English
AB Based on the theory of solidity of glass fiber-reinforced plastics (GRP), the dependence of the mech. strength of composites contg. E-glass reinforcement and metalliferous epoxy chelate polymers (MECP) on the mass of the chelate hardeners produced by the reactions of some org. salts of the transition metals (Cu, Co, Cd, Ni, Zn, Fe, Mn) with aliph. amines as the ligands is studied. The maximal values of the coeff. of solidity (S) corresponding to the maximal mech. strength of GRP can be reached when 1 mol diglycidyl ether or bisphenol A is cured by 0.14 mol of the hardeners. Anal. of the dependence of GRP strength properties on the structures of chelate hardeners showed a predominant influence of the org. salt anion and, to a lesser extent, the metal cations. To a much lesser degree, the ligands can be explained by the dependence of the adhesional strength of the "polymer-glass" system on the concn. of the polar groups (the anions and metal cations) in the polymer matrix. The dynamics of changing S as a result of the variation of the hardener content in the epoxy compns. is primarily dependent on the metal cation type. The maximal values of S correspond to Zn^{2+} and Cu^{2+} . The values obtained for the dependence of MECP properties on complex hardener structural fragments (anion, cation, and ligand) allows for preliminary evaluation of the metal chelate structures and epoxy compd. compns. necessary to produce GRP with a required set of properties.

L7 •ANSWER 27 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1992:435658 CAPLUS

DN 117:35658

TI Intersystem crossing in iron(II) coordination compounds

AU Hauser, Andreas

CS Inst. Anorg. Chem., Johannes-Gutenberg-Univ., Mainz, D-6500, Germany

SO Coordination Chemistry Reviews (1991), 111, 275-90

CODEN: CCHRAM; ISSN: 0010-8545

DT Journal

LA English

AB Due to the fact that for d6-systems there are a no. of low-lying ligand field (LF) states the relaxation from excited states of Fe(II) coordination compds. is, in general, a very fast and radiationless process. In Fe(II) spin-crossover systems, however, the zero point energy difference between the two lowest states, namely the low-spins (LS) $1A_1$ and the high-spin (HS) $5T_2$ state, is of the order of kBT, and some systems can be converted quant. to the HS state well below the thermal transition temp. by irradiating either into MLCT or LF absorption bands of the LS species, with HS \rightarrow LS relaxation rates as small as $10^{-6} s^{-1}$ at $\sim 10 K$. It is also possible to achieve a light-induced transient population of a HS state in Fe(II) LS compds., but in this case the HS \rightarrow LS relaxation rates can be larger than $10^6 s^{-1}$ even at low temps. The HS \rightarrow LS relaxation rates show strong deviations from Arrhenius kinetics with nearly temp. independent tunneling below $\sim 70 K$ and a thermally activated behavior above $\sim 100 K$. The range of 12 orders of magnitude in the low temp. tunneling rate can be understood in terms of nonadiabatic multiphonon relaxation, where in the strong coupling limit, with the Huang-Rhys parameter S much larger than the reduced energy gap p, an inverse energy gap law holds.

L7 ANSWER 28 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1992:58758 CAPLUS

DN 116:58758

TI Preparation of chelating agents for use as therapeutic, diagnostic and detoxification agents

IN Rongved, Paal; Klaveness, Jo; Dugstad, Harald

PA Cockbain, Julian Roderick Michaelson, UK; Nycomed A/S

SO PCT Int. Appl., 39 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9115466	A2	19911017	WO 1991-EP674	19910409 <--
	WO 9115466	A3	19911128		
	W: AU, CA, FI, JP, NO, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
	AU 9176619	A1	19911030	AU 1991-76619	19910409 <--
PRAI	GB 1990-7965		19900409		
	WO 1991-EP674		19910409		

OS MARPAT 116:58758

AB Title compds. [(XCHR1)2N(CHR1)nA(CHR1)mN(CHR1X)2 [A = XR1CHN:, (XR1CH)2N(R1CH)pN:, or A(CHR1)m = C-N bond; X = carboxy or a deriv. thereof or R1; R1 = H, mono-polyhydroxyalkyl, (substituted) alkoxy or alkoxyalkyl; m, n, p = 2-4; with provisos], and their metal chelates and salts, are prepd. for use as detoxification, diagnostic, and therapeutic agents (no data). N-Methylaminopropanediol (2.5 mmol) in DMF was treated with 1.2 mmol 1-(2-acetyloxyethyl)-1,5-bis(2,6-dioxomorpholino)-3-azapentane-3-acetic acid and the mixt. stirred under N for 16 h to give the corresponding ring-opened diamide/triacid, which was dissolved in MeOH satd. with NH3 and stirred overnight at ambient temp. to give 3,9-bis[N-methyl-(2,3-dihydroxypropylcarbamoylmethyl)]-6-(carboxymethyl)-4-(2-hydroxyethyl)-3,6,9-triazaundecanedioic acid (I). I was dissolved in H2O and Gd(III) oxide was added and the mixt. refluxed overnight to give Gd chelate of I (II). Pharmaceutical formulations contg. II and other chelates are given.

L7 ANSWER 29 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1992:58757 CAPLUS

DN 116:58757

TI Preparation of biological aminopolycarboxylic acid chelating agents

IN Rongved, Paal; Klaveness, Jo; Dugstad, Harald

PA Cockbain, Julian Roderick Michaelson, UK; Nycomed A/S

SO PCT Int. Appl., 43 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9115467	A1	19911017	WO 1991-EP675	19910409 <--
	W: AU, CA, FI, JP, NO, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
	AU 9176642	A1	19911030	AU 1991-76642	19910409 <--
PRAI	GB 1990-7967		19900409		
	WO 1991-EP675		19910409		

OS MARPAT 116:58757

AB Title compds. (XCHR1)2N(CHR1)nA(CHR1)mN(CHR1X)2 [A = XR1CHN:, (XR1CH)2N(R1CH)pN:, (R1CH)mA represents a C-N bond; X = HO2C or deriv. thereof, R1 = H, (substituted) alkoxy, (substituted) alkyl, R3R2NCO; R2 = H, (substituted) alkyl; R3 = (substituted) alkoxyalkyl, etc.; m, n, p = 2-4; with provisos], metal chelates and salts thereof, as therapeutic, diagnostic, and detoxification agent (no data) are prepd. 2-(Aminoethoxy)ethanol in AcNME3, was added to 1,5-bis(2,6-dioxomorpholino)-3-azapentane-3-acetic acid, the soln. stirred overnight and a soln. of ether/chloroform (1:1 ratio) added to give 6-(carboxymethyl)-3,9-bis(5-hydroxy-3-oxapentylcarbamoylmethyl)-3,6,9-triazaundecane diacid (I). I dissolved in H2O was added to Gd(III) oxide, and the mixt. refluxed overnight to give Gd I chelate. Formulations comprising the title chelates are given.

L7 ANSWER 30 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1992:50227 CAPLUS

DN 116:50227
 TI Complexes of divalent metals with ethylenediaminetriacetatoacetic acid ligand $[M(H_2O)_6][H_2O](Hedta)]2.2H_2O$. I. Co, Mg, Ni and Zn
 AU Aroztegui Trenchs, Montserrat; Calpena Capmany, Anna Cristina; Sanchez Gimeno, Roser; Vidal Bosch, Pere; Oliva Gimeno, Jose Ignacio
 CS Dep. Farm., Univ. Barcelona, Spain
 SO Circular Farmaceutica (1943-1992) (1991), 49(1), 25-36
 CODEN: CIFA33; ISSN: 0366-6425
 DT Journal
 LA Spanish
 AB $M_3(HL)2.10H_2O$ ($M = Zn, Ni, Co, Mg$, $H_4L = EDTA$) were prepd. from the metal carbonates. They were characterized by electronic spectra, thermal dehydrations and x-ray crystal structures. All are monoclinic and their lattice parameters are given. Data reveal the compds. may be formulated as $[M(H_2O)_6][M(H_2O)(HL)]2.2H_2O$ with the ligand pentadentate by 2 N and 3 O atoms. One acetate arm is free and protonated. Crystal field parameters are given for the Co and Ni complexes.

L7 ANSWER 31 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1992:33238 CAPLUS
 DN 116:33238
 TI Studies on complexes of divalent metals with ethylenediaminetriacetatoactate as ligands $[M(H_2O)_4][M(H_2O)(HEDTA)]2.4H_2O$. II. Manganese and cadmium
 AU Aroztegui Trenchs, Montserrat; Calpena Capmany, Anna Cristina; Sanchez Gimeno, Roser; Herrera Corominas, Julia; Oliva Gimeno, Jose Ignacio
 CS Dep. Farm., Univ. Barcelona, Barcelona, Spain
 SO Circular Farmaceutica (1943-1992) (1991), 49(2), 131-8
 CODEN: CIFA33; ISSN: 0366-6425
 DT Journal
 LA Spanish
 AB $Mn_3(HL)2.10H_2O$ and $Cd_3(HL)2.10H_2O$ ($H_4L = EDTA$) were prepd. and characterized by thermal decompn. and x-ray crystal structures. Both are monoclinic and their lattice parameters are given. The compds. contain distinct $[M(H_2O)_4]^{2+}$ and $[M(H_2O)(HL)]^-$ coordinations ($M = Cd, Mn$).

L7 ANSWER 32 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1991:218628 CAPLUS
 DN 114:218628
 TI Structures of two zinc(2+) complexes with two tetraaza macrocyclic tetraacetates
 AU Riesen, Andreas; Zehnder, Margareta; Kaden, Thomas A.
 CS Inst. Inorg. Chem., Univ. Basel, Basel, CH-4056, Switz.
 SO Acta Crystallographica, Section C: Crystal Structure Communications (1991), C47(3), 531-3
 CODEN: ACSCEE; ISSN: 0108-2701
 DT Journal
 LA English
 AB (1,4,7,10-Tetraazacyclododecane- N,N',N'',N''' -dihydrogentetraacetato)zinc (I) is, orthorhombic, space group $Pccn$, with a 9.354(4), b 15.294(7), and c 13.114(4) .ANG.; .ANG.3 $dc = 1.656$ for $Z = 4$; final $R = 0.048$ for 1620 reflections. . (1,4,8,11-Tetraazacyclotetradecane- N,N',N'',N''' -dihydrogentetraacetato)zinc tetrahydrate, (II) is monoclinic, space group $P2_1/c$ with a 8.695(2), b 15.456(7), c 8.993(2) .ANG., and .beta. 90.46(2).degree.; .ANG.3, $dc = 1.561$ for $Z = 2$; final $R = 0.029$ for 2267 reflections. At. coordinates are given. In both Zn^{2+} complexes the metal ion is coordinated by 4 nitrogens of the macrocycle and 2 carboxylate O atoms. The other 2 carboxylate moieties are protonated and are not involved in coordination, but form H bonds. Due to the ring size of the macrocycle, the geometry around the Zn^{2+} is, however, different in the 2 complexes. In I the Zn^{2+} is in a cis-octahedral arrangement, whereas in II a trans-octahedral coordination is obsd. with the Zn^{2+} in the plane of the 4 nitrogens of the macrocycle. The configuration of the macrocycle is cis-I and trans-III for I and II, resp.

L7 ANSWER 33 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1991:34636 CAPLUS
 DN 114:34636
 TI Transannular oscillation of metal centers in the pendant arm macrocyclic complex [1,4,8,11-tetrakis(2-hydroxyethyl)-1,4,8,11-tetraazacyclotetradecane]mercury(II) and its lead(II) analog. NMR study of the carbon-13 natural abundance and specifically enriched complexes
 AU Clarke, Philip; Lincoln, Stephen F.; Wainwright, Kevin P.
 CS Dep. Phys. Inorg. Chem., Univ. Adelaide, Adelaide, 5001, Australia
 SO Inorganic Chemistry (1991), 30(1), 134-9
 CODEN: INOCAJ; ISSN: 0020-1669
 DT Journal
 LA English
 AB A ^{13}C NMR study of [1,4,8,11-tetrakis(2-hydroxyethyl)-1,4,8,11-tetraazacyclotetradecane]mercury(II) and its lead(II) analog $[\text{M}(\text{THEC})]^{2+}$ ($\text{M} = \text{Hg}, \text{Pb}$), in CD_3OD shows that the most probable structure of these complexes in soln. incorporates the 1,4,8,11-tetraazacyclotetradecane ring in the trans III configuration with the metal center above the tetraaza plane and trigonal-prismatically coordinated by four ring nitrogens and two hydroxyethyl pendant arms attached to either end of the same 1,3-diaminopropane moiety. Dynamic ^{13}C NMR studies of $[\text{M}(\text{THEC})]^{2+}$ are consistent with a rapid pairwise intramol. exchange of the hydroxyethyl arms between mono- and bidentate coordination simultaneously with the oscillation of $\text{M}(\text{II})$ through the macrocyclic annulus of THEC. This pairwise exchange of the hydroxyethyl arms is characterized by $k(298.2 \text{ K}) = 3130 \pm 120$ and $11,200 \pm 220 \text{ s}^{-1}$, heats $\Delta H = 38.0 \pm 0.6$ and $45.4 \pm 0.3 \text{ kJ/mol}$, and entropies $\Delta S = -50.6 \pm 2.1$ and $-15.2 \pm 1.1 \text{ J/K.mol}$, for $\text{M} = \text{Hg}$ and Pb , resp.

L7 ANSWER 34 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1991:16559 CAPLUS
 DN 114:16559
 TI Interaction of ethambutol with transition metal ions in solution: formation constants and stereochemical configurations of the copper(II), nickel(II), cobalt(II) and zinc(II) complexes and underlying biological implications
 AU Bhattacharyya, R. G.; Paul, U. K.; Chatterjee, A. B.; Bag, S. P.
 CS Dep. Chem., Jadavpur Univ., Calcutta, 700 032, India
 SO Indian Journal of Chemistry, Section A: Inorganic, Physical, Theoretical & Analytical (1990), 29A(10), 986-95
 CODEN: IJCADU; ISSN: 0376-4710
 DT Journal
 LA English
 AB Ethambutol (ETB), reacts with aq. Cu^{2+} , Co^{2+} and Ni^{2+} at pH 11 producing $[\text{M}(\text{H}_2\text{O})_4\text{ETB}]^{2+}$ ($\text{M} = \text{Cu}, \text{Co}$) and $[\text{Ni}_2(\text{OH})_2(\text{H}_2\text{O})_4(\text{ETB})_2]^{2+}$. $\text{Ni}(\text{II})$ at pH 9 forms $[\text{NiL}_4\text{ETB}]^{2+}$ ($\text{L} = \text{H}_2\text{O}, \text{NH}_3$ depending on whether NaOH or NH_4OH is used to maintain the pH). Spectrophotometric and potentiometric studies suggest that metal-ligand [ETB] formation const. is highest in the case of $\text{Cu}(\text{II})$, and ΔG accompanying the Cu -ETB complex formation is the most neg. The $\text{Cu}(\text{II})$, $\text{Ni}(\text{II})$ and $\text{Co}(\text{II})$ complexes have pseudooctahedral structure, according to their soln. magnetic susceptibility and ligand field spectra. Dq (ETB) is exceedingly large for $\text{Cu}(\text{II})$, followed by that for $\text{Ni}(\text{II})$ and $\text{Co}(\text{II})$. The soln. data were corroborated by isolating the BPh_4 salts of the complex cations, viz., $[\text{M}(\text{H}_2\text{O})_4\text{ETB}](\text{BPh}_4)_2$ ($\text{M} = \text{Cu}, \text{Co}, \text{Ni}$), $[\text{Ni}(\text{NH}_3)_4\text{ETB}](\text{BPh}_4)_2$, $[\text{Zn}(\text{H}_2\text{O})_2(\text{ETB})](\text{BPh}_4)_2$ and $[\text{Ni}_2(\text{OH})_2(\text{H}_2\text{O})_4(\text{ETB})_2](\text{BPh}_4)_2$. These salts were characterized by elemental anal., molar cond., magnetic susceptibility, EPR (for $\text{Cu}(\text{II})$ complex), IR and UV-visible spectroscopy. The mode of coordination of ETB is supported by the ^1H NMR data on $\text{Zn}(\text{II})$ complex. This in vitro study is quite consistent with the idea that ETB treatment (for some resistant strains of *Mycobacterium tuberculosis*) depletes Cu^{2+} in the physiol. system.

L7 ANSWER 35 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1990:477986 CAPLUS
 DN 113:77986
 TI Suicidal inactivation of iron porphyrins during trans-hex-2-ene oxidation: first isolation and characterization of N-alkylporphyrins with a N-CHR-CHR'OH structure
 AU Artaud, Isabelle; Gregoire, Nathalie; Mansuy, Daniel
 CS Lab. Chim. Biochim. Pharmacol. Toxicol., Univ. Rene Descartes, Paris, 75270, Fr.
 SO New Journal of Chemistry (1989), 13(8-9), 581-6
 CODEN: NJCHE5; ISSN: 0398-9836
 DT Journal
 LA English
 OS CASREACT 113:77986
 AB The oxidn. of trans-hex-2-ene by PhIO catalyzed by meso-tetrakis(p-chlorophenyl)porphyriniron(III) chloride causes an irreversible transformation of the catalyst which leads, after acidic demetallation, to two isomeric N-alkylporphyrins derived from the two possible syn addns. of an O atom and of a pyrrole N to the alkene double bond. These two isomers, which are among the very few examples of N-alkylporphyrins where the pyrrole N is bound to a disubstituted carbon, were characterized by UV-visible and 1H-NMR spectroscopy (including 2D-NMR techniques) and mass spectrometry. These results show that heme N-alkylation which has been obsd. in competition with epoxidn. in cytochrome P 450- or iron-porphyrin-catalyzed oxidn. of monosubstituted alkenes also occurs with 1,2-disubstituted alkenes.

L7 ANSWER 36 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1990:228421 CAPLUS
 DN 112:228421
 TI Carbon-13 and cadmium-113 nuclear magnetic resonance evidence for a novel transannular oscillation of cadmium(II) in the pendant arm macrocyclic complex [1,4,8,11-tetrakis(2-hydroxyethyl)-1,4,8,11-tetraazacyclotetradecane]cadmium(II)
 AU Clarke, Philip; Hounslow, Andrea M.; Keough, Rebecca A.; Lincoln, Stephen F.; Wainwright, Kevin P.
 CS Dep. Phys. Inorg. Chem., Univ. Adelaide, Adelaide, Australia
 SO Inorganic Chemistry (1990), 29(10), 1793-7
 CODEN: INOCAJ; ISSN: 0020-1669
 DT Journal
 LA English
 AB A 13C NMR study of [1,4,8,11-tetrakis(2-hydroxyethyl)-1,4,8,11-tetraazacyclotetradecane]cadmium (II), [Cd(THEC)]2+, in CD3OD shows that the most probable structure for [Cd(THEC)]2+ incorporates the 1,4,8,11-tetraazacyclotetradecane ring in the trans III configuration. In this structure Cd(II) is above the tetraaza plane and is trigonal-prismatically coordinated by four ring nitrogens and two hydroxyethyl pendant arms attached to either end of the same 1,3-diaminopropane moiety. The 13C CPMAS NMR spectrum of solid [Cd(THEC)]2+ is also consistent with this structure. Dynamic 13C NMR studies of natural abundance [Cd(THEC)]2+ and of [Cd(THEC)]2+ in which both carbons of each of the hydroxyethyl arms are 99 atom % enriched in 13C are consistent with a rapid oscillation of Cd(II) through the macrocyclic annulus of THEC. The 13C-enriched hydroxyethyl arms are characterized by 13C AB quartets under conditions of slow exchange but show a novel coalescence to a singlet under fast-exchange conditions consistent with the relative chem. shifts of the methylene carbons of the hydroxyethyl arm being reversed when it changes from the mono- to the bidentate coordination state. The pairwise exchange of the hydroxyethyl arm between the monodentate and bidentate environments is characterized by $k(298.2\text{ K}) = 34200 \pm 1800\text{ s}^{-1}$, $\Delta H_{\text{thermod.}} = 44.00 \pm 0.56\text{ kJ mol}^{-1}$, and $\Delta S_{\text{thermod.}} = -10.6 \pm 2.2\text{ J K}^{-1}\text{ mol}^{-1}$. 13C and 113Cd NMR spectra show that intermol. THEC and Cd(II) exchange on [Cd(THEC)]2+ is a much slower process.

L7 ANSWER 37 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1989:633674 CAPLUS

DN 111:233674

TI Preparation of chelates of aminopolycarboxylates as therapeutic and diagnostic agents

IN Berg, Arne; Almen, Torsten; Thomassen, Terje; Klaveness, Jo; Rongved, Pal

PA Nycomed A/S, Norway

SO Eur. Pat. Appl., 42 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 299795	A2	19890118	EP 1988-306520	19880715 <--
	EP 299795	A3	19890802		
	EP 299795	B1	19920318		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	WO 8900557	A1	19890126	WO 1988-GB572	19880715 <--
	W: AU, DK, FI, GB, HU, JP, NO, SU, US				
	AU 8819980	A1	19890213	AU 1988-19980	19880715 <--
	AU 617338	B2	19911128		
	JP 02504269	T2	19901206	JP 1988-505904	19880715 <--
	JP 2833766	B2	19981209		
	HU 54621	A2	19910328	HU 1988-4196	19880715 <--
	EP 466200	A1	19920115	EP 1991-113755	19880715 <--
	EP 466200	B1	19960424		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	AT 73761	E	19920415	AT 1988-306520	19880715 <--
	ES 2033433	T3	19930316	ES 1988-306520	19880715 <--
	HU 64950	A2	19940328	HU 1993-2702	19880715 <--
	AT 137228	E	19960515	AT 1991-113755	19880715 <--
	ES 2086445	T3	19960701	ES 1991-113755	19880715 <--
	RU 2073005	C1	19970210	RU 1988-4743079	19880715 <--
	ZA 8805178	A	19890426	ZA 1988-5178	19880718 <--
	DK 9000074	A	19900111	DK 1990-74	19900111 <--
	NO 9000192	A	19900308	NO 1990-192	19900115 <--
	NO 179973	B	19961014		
	NO 179973	C	19970122		
	AU 9183431	A1	19911107	AU 1991-83431	19910829 <--
	AU 640263	B2	19930819		
PRAI	GB 1987-16778		19870716		
	GB 1987-16914		19870717		
	EP 1988-306520		19880715		
	HU 1988-4196		19880715		
	WO 1988-GB572		19880715		

OS MARPAT 111:233674

AB XCHR1NZ(CHR2)nA(CHR3)mNZ1CHR4X1 [I; R1-R9 = H, hydroxyalkyl, (hydroxylated) alkoxy, alkoxyalkyl; A, A1 = O, S, NY; ACHR1 = C-N bond; X-X4 = carboxy (deriv.), R1; Y = (CHR5)p N(CHR6X2)2, CHRX3; Z = CHR7X4; groups Z together = (CHR8)qA1(CHR9)r; n, m, p, q, r = 2-4], useful as chelating agents for prepn. of diagnostic and therapeutic agents (no data), were prepd. N(CH2CO2H)3, H2SO4, and EtOH were refluxed 4 h to give N(CH2CO2Et)3, which in EtOH was added dropwise to hot aminopropanediol. The mixt. was stirred 3 h at 120.degree. to give an amide. The latter in DMF was stirred with tosic acid and MeC(OMe)2Ph at 60.degree. and 200 mbar to give a ketal which was treated with LiAlH4 in refluxing THF followed by treatment with BrCH2CO2Na in MeOH/H2O at 40.degree. and stirring overnight with HBr in H2O/acetone to give N,N,N-tris-[(N'-carboxymethyl-N'-2,3-dihydroxypropyl)-2-aminoethyl]amine. The Gd(III) chelate of the latter was prepd. by heating with Gd2O3 in H2O at 95.degree. overnite. A soln. contg. 6.9 g of the chelate and 20 mL of H2O was prepd.

L7 ANSWER 38 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1989:429133 CAPLUS
DN 111:29133
TI Mixed ligand nickel or zinc nitrilotriacetate or ethylenediaminetetraacetate complexes with hydroquinone
AU Rostunov, Yu. V.; Barkhanova, N. N.; Fridman, A. Ya.; Dyatlova, N. M.
CS Vses. Nauchno-Issled. Inst. Khim. Reakt. Osobo Chist. Veshchestv, USSR
SO Koordinatsionnaya Khimiya (1989), 15(4), 519-23
CODEN: KOKHDC; ISSN: 0132-344X
DT Journal
LA Russian
AB Stability consts. were detd. pH-metrically for Ni(II) or Zn mixed ligand complexes with NTA (H3L) or EDTA (H4Y) and hydroquinone (HQ) at ionic strength 1.5(NH4Cl) and 293 K. Electronic spectra of these mixed complexes (MLQ2- or MYQ3-) were detd. in soln. The complexes were isolated for an IR spectral study of their structures by reactions of the type Na[ML](Na2[MY]) + HQ + 2Na2SO3 .fwdarw. Na2[MLQ](Na3[MYQ]).Na2SO3.NaHSO3. The solid complexes were obtained by evapn. and crystn. from aq. alc. solns. and the IR spectra were detd. for complex suspensions in mineral oil or hexachlorobutadiene.

L7 ANSWER 39 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1989:415614 CAPLUS
DN 111:15614
TI Bimetallic compounds of trans-cyclohexane-1,2-diamine-NNN'N'-tetraacetate (cdta). Part 3. Structural and magnetic characterization of the dinuclear [M(OH2)5][M'(cdta)].H2O (M,M' = Ni,Ni; Mn,Ni; Mn,Cu; Co,Ni; or Co,Cu) and the tetranuclear [M(OH2)4]M'(cdta)(OH2)].4H2O (M,M' = Zn,Zn; Zn,Co; Co,Co; or Mn,Co) complexes
AU Fuertes, Amparo; Miravittles, Carlos; Escriva, Emilio; Coronado, Eugenio; Beltran, Daniel; Padel, Lilyane
CS Inst. Cienc. Mater. Barcelona, Barcelona, 08028, Spain
SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999) (1989), (5), 863-71
CODEN: JCDTBI; ISSN: 0300-9246
DT Journal
LA English
AB The Co,Cu title compd. (I) is orthorhombic, space group Pbc21, with a 10.878(5), b 11.167(5), and c 17.446(14) .ANG.; dc = 1.80 for Z = 4. The Zn,Zn title compd. (II) is monoclinic, space group P21/n, with a 9.702(2), b 11.757(2), c 20.980(5) .ANG., and .beta. 95.61(2).degree.; dc = 1.77 for Z = 4. The Co,Zn title compd. (III) is monoclinic, space group P21/n, with a 9.731(9), b 11.783(2), c 21.031(9) .ANG., and .beta. 95.40(1).degree.; dc = 1.74 for Z = 4. The final R's = 0.056, 0.098, and 0.041 for I, II, and III, resp. At. coordinates are given. The structure of I consists of dinuclear entities constructed from cationic Co(OH2)52+ and anionic Cu(cdta)2- mols. which are linked through a bridging carboxylate group from the cdta ligand. In II and III, the species M(2)(OH2)42+ and M(1)(cdta)(OH2)2-, sharing 2 O atoms from different carboxylate groups, alternate to form tetranuclear entities. The magnetic properties at 1-100 K of the title compds. are discussed by assuming a Heisenberg or Ising exchange coupling between the 2 metal ions with distinct Lande factors and local distortion parameters. All the compds show antiferromagnetic behavior at low temps., with exchange coupling parameters ranging from -0.8 to -8.8 cm-1.

L7 ANSWER 40 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1989:129997 CAPLUS
DN 110:129997
TI Comparative mobilization of lead by chelating agents
AU Xu, Zhaofa; Jones, Mark M.
CS Dep. Public Health, China Med. Univ., Shenyang, Peop. Rep. China
SO Toxicology (1988), 53(2-3), 277-88
CODEN: TXCYAC; ISSN: 0300-483X
DT Journal

LA English
AB The relative abilities of .apprx.20 chelating agents to act as antagonists for acute and chronic Pb poisoning were examd. in the mouse. The acute LD50 for Pb acetate trihydrate was 135.3 mg Pb/kg for i.p. injection. The relative efficacy of chelating agents to reduce liver, kidney, spleen, bone, and brain levels of Pb was detd. The movement of Pb from the liver to the bone was followed during the first 7 days postinjection and resulted in appreciable changes in the Pb levels of the organs from day to day during this entire period. Of the compds. examd., the ones which were most effective in mobilizing Pb under various conditions included meso-2,3-dimercaptosuccinic acid (DMSA), sodium 2,3-dimercaptopropane-1-sulfonate, Na2CaEDTA, trisodium zinc triethylenetetraminehexaacetate, dicalcium ethylenediaminetetra(methylenephosphonate) and di-Et dimercaptosuccinate, and BAL.

L7 ANSWER 41 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1989:50175 CAPLUS
DN 110:50175
TI 1,3-Bis(2,5,8,11-tetraazaundecyl)benzene (MXTRIEN): synthesis, binucleating chelating tendencies, and formation and thermal degradation of its cobalt dioxygen complex
AU Menif, Rached; Martell, Arthur E.
CS Dep. Chem., Texas A and M Univ., College Station, TX, 77843, USA
SO Inorganic Chemistry (1989), 28(1), 116-22
CODEN: INOCAJ; ISSN: 0020-1669

DT Journal
LA English
AB Prepn. and potentiometric equil. studies of the stabilities of the complexes of 1,3-bis(2,5,8,11-tetraazaundecyl)benzene (MXTRIEN) with Cu(II), Co(II), Ni(II), and Zn(II) are reported. Equil. consts. are detd. for the formation of mononuclear and dinuclear chelates of these metal ions, as well as several protonated and hydroxo chelates. O2 combines with the Co(II) complex to form a stable dibridged .mu.-hydroxo .mu.-peroxo dinuclear complex. The autoxidn. of the Co(II) complex through the formation of the O2 complex results in a metal-centered oxidn. to form the CoIII2 chelate and H2O2.ide. The 1st step of the autoxidn. reaction is 1st-order with respect to the concn. of both the dioxygen complex and OH-.

L7 ANSWER 42 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1988:544476 CAPLUS
DN 109:144476
TI The synthesis and biological activity of some potentially fungicidal zinc ethylenebis(dithiocarbamate):amine complexes
AU Clifford, David P.; Carson, Chrislyn
CS Letcombe Lab., Dow Chem., Letcombe Regis/Wantage/Oxon, UK
SO Pesticide Science (1988), 23(2), 93-102
CODEN: PSSCBG; ISSN: 0031-613X

DT Journal
LA English
AB Thirty-one complexes of zinc ethylenebis(dithiocarbamate), zineb, were synthesized and evaluated in comparison with zineb and mancozeb across a broad range of pathogens (e.g., apple mildew, grape downy mildew, apple scab, wheat leaf rust, barley mildew, verticillium wilt, tobacco diseases). The activity of zineb was greatly potentiated and its persistence increased against several pathogens, particularly Puccinia recondita. The generation of the dithiocarbamate ion from zineb by excess amine provided a convenient anal. procedure for zineb anal. In general, amines contg. no OH group and for which complex ring formation was not possible gave active compds. against all pathogens; morpholine complexes showed good and persistent activity against leaf rust.

L7 ANSWER 43 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1988:465873 CAPLUS

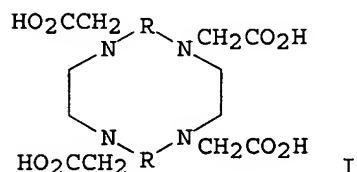
DN 109:65873
 TI Thermally-induced phase transition of zinc(II) diamine complexes in the solid state
 AU Roy, Sukumar; Ghosh, Ashutosh; Chaudhuri, Nirmalendu Ray
 CS Dep. Inorg. Chem., Indian Assoc. Cultiv. Sci., Calcutta, 700 032, India
 SO Thermochemica Acta (1988), 127, 329-35
 CODEN: THACAS; ISSN: 0040-6031
 DT Journal
 LA English
 AB $\text{ZnLCl}_2 \cdot 0.5\text{H}_2\text{O}$ and $\text{ZnL}_2\text{X}_2 \cdot n\text{H}_2\text{O}$ [$\text{L} = \text{N}-2(\text{hydroxyethyl})-1,2\text{-ethanediamine}$; $\text{X} = \text{Br}$, 0.5SO_4 , 0.5SeO_4 and $n = 0.5-2$] were prepd. and thermal studies were carried out in the solid state. $\text{ZnLCl}_2 \cdot 0.5\text{H}_2\text{O}$ and $\text{ZnL}_2\text{Br}_2 \cdot 0.5\text{H}_2\text{O}$ show endothermic reversible phase transitions ($135.0-152.0^\circ\text{C}$; $\Delta H = 1.6 \text{ kJ mol}^{-1}$ and $127.0-144.5^\circ\text{C}$; $\Delta H = 10.4 \text{ kJ mol}^{-1}$, resp.) after dehydration. $\text{ZnL}_2\text{SO}_4 \cdot 2\text{H}_2\text{O}$ is hydrated at 100°C . and on further heating undergoes an exothermic irreversible phase transition ($109.5-146.0^\circ\text{C}$; $\Delta H = -9.5 \text{ kJ mol}^{-1}$), whereas $\text{ZnL}_2\text{SeO}_4 \cdot \text{H}_2\text{O}$ 1st undergoes dehydration at 134°C . and then an endothermic irreversible phase transition occurs ($141.5-171.5^\circ\text{C}$; $\Delta H = 14.2 \text{ kJ mol}^{-1}$).

L7 ANSWER 44 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1988:48087 CAPLUS
 DN 108:48087
 TI Design of ordered bimetallic complexes. Part 2. Trans-1,2-cyclohexanediaminetetraacetate bimetalates
 AU Fuertes, Amparo; Escriva, Emilio; Munoz, Carmen; Alamo, Jaime; Beltran-Porter, Aurelio; Beltran-Porter, Daniel
 CS Inst. Cienc. Mater., Barcelona, 08020, Spain
 SO Transition Metal Chemistry (Dordrecht, Netherlands) (1987), 12(1), 62-8
 CODEN: TMCHDN; ISSN: 0340-4285
 DT Journal
 LA English
 AB Knowledge of the kinetic and thermodyn. behavior of aq. solns. contg. 2 divalent cations and trans-1,2-cyclohexanediaminetetraacetic acid (H_4L) was used to design synthetic pathways to ordered bimetallic complexes. $[\text{M}(\text{H}_2\text{O})_m][\text{M}_1\text{L}(\text{H}_2\text{O})_n] \cdot x\text{H}_2\text{O}$ ($\text{M} = \text{M}_1 = \text{Cu, Ni, Zn, Co}$; $\text{M} = \text{Zn, Mn}$, $\text{M}_1 = \text{Cu, Co, Ni}$; $\text{M} = \text{Ni, Co}$, $\text{M}_1 = \text{Cu}$; $\text{M} = \text{Mg, Co, Cu}$, $\text{M}_1 = \text{Ni}$; $\text{M} = \text{Ni}$, $\text{M}_1 = \text{Co}$; $\text{M} = \text{Mg}$, $\text{M}_1 = \text{Zn}$) were prepd. Electronic spectral assignments and crystal field parameters are reported for 14 complexes.

L7 ANSWER 45 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1987:416646 CAPLUS
 DN 107:16646
 TI Coordination complexes of drugs - preparation and characterization of metal complexes of primaquine
 AU Wasi, Nadira; Singh, H. B.
 CS Dep. Chem., Delhi Univ., Delhi, 110007, India
 SO Synthesis and Reactivity in Inorganic and Metal-Organic Chemistry (1987), 17(1), 129-41
 CODEN: SRIMCN; ISSN: 0094-5714
 DT Journal
 LA English
 AB $\text{ML}_2\text{Cl}_2 \cdot n\text{H}_2\text{O}$ ($\text{L} = \text{primaquine}$; $\text{M} = \text{Cd, Cu, Pd, Pt, Hg, Sn}$, $n = 0$; $\text{M} = \text{Ni, Mn, Zn}$, $n = 2$; $\text{M} = \text{Co}$, $n = 5$), $\text{M}_1\text{L}_3\text{Cl}_3$ ($\text{M}_1 = \text{Cr, Fe, Au, Rh}$), VOL_2SO_4 , and AgL_2NO_3 were prepd. IR spectral studies suggest that primaquine acts as a bidentate ligand.

L7 ANSWER 46 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1987:187824 CAPLUS
 DN 106:187824
 TI Synthesis of metal complexes of antimalarial drugs and in vitro evaluation of their activity against Plasmodium falciparum
 AU Wasi, Nadira; Singh, H. B.; Gajanana, A.; Raichowdhary, A. N.

- CS Dep. Chem., Delhi Univ., Delhi, 110007, India
 SO Inorganica Chimica Acta (1987), 135(2), 133-7
 CODEN: ICHAA3; ISSN: 0020-1693
- DT Journal
 LA English
- AB Thirty-two complexes of 2 well-known antimalarials, amodiaquine and primaquine, with VO(II), Cr(III), Fe(III), Cu(II), Co(II), Ni(II), Zn(II), Cd, Hg(II), Rh(III), Pd(II), Au(III), Ag(I), Mn(II), Sn(II) and Pt(II) were prepd., characterized and screened by an in vitro microtechnique for their schizonticidal activity with a view to search for a more effective agent. The antiparasitic activity of the 2 drugs is independent of their coordination to any metal.
- L7 ANSWER 47 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1987:167683 CAPLUS
 DN 106:167683
- TI Synthetic and solution studies on metal complexes of N,N,N',N'-tetrakis(2-carbamoylethyl)ethylenediamine
- AU Hay, Robert W.; Pujari, Mahesh P.; Govan, Norman; Perotti, Angelo
 CS Chem. Dep., Univ. Stirling, Stirling, FK9 4LA, UK
 SO Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999) (1986), (12), 2539-44
 CODEN: JCDBTI; ISSN: 0300-9246
- DT Journal
 LA English
- AB Tetrakis(2-carbamoylethyl)ethylenediamine (H2L) was prepd. by Michael addn. of ethylenediamine to acrylamide. ML (M = Cu, Ni, and Pd) and M1(H2L)Cl_n.xH₂O (M1 = Fe, Mn, Zn, Cd, Hg, n = 2; M1 = La, n = 3) were prepd. and characterized in the solid state by elemental anal., molar cond., and spectral (IR, visible) methods. The stepwise protonation of H2L was studied by potentiometric titrn., giving log K₁ = 7.20(1) and log K₂ = 3.25(2) at 25.degree. and I = 0.1 mol dm⁻³ (NaClO₄). Titrn. data for the molar ratio H2L/M = 1:1 (M = Cu, Ni, or Pd) were fitted to the stepwise equil. and the corresponding log .beta. values are reported.
- L7 ANSWER 48 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1987:112579 CAPLUS
 DN 106:112579
- TI Metal complexes of macrocyclic ligands. Part XXIII. Synthesis, properties, and structures of mononuclear complexes with 12- and 14-membered tetraazamacrocyclic-N,N',N'',N'''-tetraacetic acids
- AU Riesen, Andreas; Zehnder, Margareta; Kaden, Thomas A.
 CS Inst. Anorg. Chem., Univ. Basel, Basel, CH-4056, Switz.
 SO Helvetica Chimica Acta (1986), 69(8), 2067-73
 CODEN: HCACAV; ISSN: 0018-019X
- DT Journal
 LA English
 GI



- AB I (R = (CH₂)₂ (H4dota, H4L), (CH₂)₃ (H4teta)) form with Ni²⁺, Cu²⁺, and Zn²⁺ (M₂⁺) MLH₂ and M' [ML], M' being an alk. earth ion. The structures of Ni(H₂dota) and Cu(H₂dota) were solved by x-ray structure anal. The metal ions are in a distorted octahedral geometry coordinated by 4 amino N-atoms and 2 carboxylates. In the case of Cu²⁺, the distortions are more

pronounced than for Ni²⁺ indicating that the Jahn-Teller effect is operating. Starting from these 2 structures, the coordination geometry of the other complexes is discussed using visible and IR spectra.

L7 ANSWER 49 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1987:62427 CAPLUS
 DN 106:62427
 TI Interaction of chelating agents, ferridextran and zinc with indium in mice.
 AU Eybl, V.; Koutensky, J.; Sykora, J.; Mertl, F.
 CS Med. Fac., Charles Univ., Plzen, Czech.
 SO Acta Pharmacologica et Toxicologica, Supplement (1986), 59(7),
 475-7
 CODEN: APTSAI; ISSN: 0065-1508
 DT Journal
 LA English
 AB I.p. injection of InCl₃ followed by s.c. injection of chelators (5:1) decreased In toxicity in the series CaNa₃DTPA [12111-24-9] = meso-2,3-dimercaptosuccinic acid (DMSA) [304-55-2] > DMPS [4076-02-2] = ZnNa₃DTPA [11082-38-5]. I.p. injection of the chelators (10:1) 24 h after i.v. 114mInCl₃ injection decreased whole-body retention of In; DMSA was most effective. Fe dextran [9004-66-4] had a prophylactic effect in InCl₃ poisoning in mice; it decreased the In content in whole body, liver, digestive tract, and blood but increased In content in the kidney. This may be due to In binding by the Fe dextran and excretion of this complex. The pretreatment of mice with ZnCl₂ decreased In toxicity but increased In retention in whole body and all organs except the kidney, where In content decreased. This may be due to metallothionein induction by the Zn pretreatment.

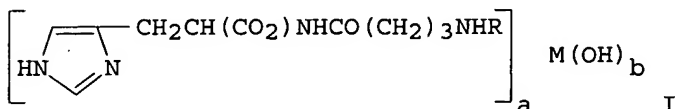
L7 ANSWER 50 OF 134 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1987:12968 CAPLUS
 DN 106:12968
 TI Homocarnosine or acylhomocarnosine salts
 IN Takaya, Masahiro
 PA Hamari Chemicals, Ltd., Japan
 SO Eur. Pat. Appl., 23 pp.
 CODEN: EPXXDW

DT Patent
 LA English

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	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 192317	A1	19860827	EP 1986-300076	19860107 <--
	EP 192317	B1	19900228		
	R: BE, CH, DE, FR, GB, IT, LI, NL, SE				
	CA 1261850	A1	19890926	CA 1985-498656	19851227 <--
	JP 62111969	A2	19870522	JP 1986-7647	19860117 <--
	JP 07064824	B4	19950712		
PRAI	JP 1985-8243		19850119		

GI



AB The title compds. (I; R = H, acyl; a = 1-3; M = Al, Zn; b = 0-2), having antiulcer and wound healing-promoting activity, were prepd. Thus, to L-homocarnosine in MeOH was added ZnCl₂, H₂O, and MeOH to give L-homocarnosine Zn (1:1) (II). In pyloric ligation-induced ulcers in rats, II showed 46.2% inhibition compared to 0 and 6.2% for no drug and

L-homocarnosine, resp.

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